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Novel Nanostructured Materials for Hydrogen Storage

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The United States Department of Energy's (DOE's) Office of Energy Efficiency and Renewable Energy and the Office of Basic Sciences have concluded that hydrogen storage is a cornerstone technology for implementing a hydrogen energy economy. However, significant scientific advancement is still required if a viable on-board storage technology is to be developed. For example, an adsorption process for on-board vehicular storage will require a hydrogen binding energy between ∼20-60 kJ/mol to allow for near-room temperature operation at reasonable pressures. Typically, non-dissociative physisorption due purely to van der Waals forces involves a binding energy of only ∼ 4 kJ/mol, whereas a chemical bond is ∼ 400 kJ/mol. The desired binding energy range for vehicular hydrogen storage therefore dictates that molecular H_2 be stabilized in an unusual manor. Hydrogen adsorption has been observed with a binding energy of ∼ 50 kJ /mol on carbon multi-wall nanotubes (MWNTs) containing iron nanoparticles at their tips. However, hydrogen adsorption at near ambient conditions is neither anticipated nor observed on either purified MWNTs or iron nanoparticles by themselves. Recent theoretical studies have shown that an iron adatom forms a complex with a C_{36} fullerene and shares charge with four carbon atoms of a bent five-membered ring in the C_{36} molecule. Three H_2 ligands then also coordinate with the iron forming a stable 18-electron organo-metallic complex. Here the binding energy of the molecular hydrogen ligands is ∼ 43 kJ /mol. It is believed that a similar interaction may be occurring for MWNTs containing iron nanoparticles. However, a more optimized material must be produced in order to increase the hydrogen capacity. Iron has also been predicted to complex with all twelve of the five-membered rings in C_{60} with a binding energy of ∼42 kJ/mol and an H_2 capacity of 4.9 wt.%. Further, Scandium has been shown to complex with the twelve five-membered rings in C_{60} with a binding energy of ∼42 kJ/mol and an H_2 capacity of 8.7 wt.%. These theoretical findings as well as experimental efforts to synthesize organo-metallic fullerene complexes for vehicular hydrogen storage applications will be discussed in detail.